REAXYSFILESUB

Subject Coverage

Extensive chemistry content:

- All types organic and inorganic substances, including alloys, coordination compounds, minerals, mixtures, polymers, and salts
- Properties and reaction data

File Type

Structure

Features

Alerts (SDIs)	Not available		
CAS Registry Number® Identifiers	☑	Structures	☑
SLART	☑		

Record Content

Substance Identification (Chemical Names, Molecular Formulas, etc.)

File Size

About 57 million records (02/2026)

Coverage

1771- present

Updates

Twice a week

Language

English

Database Producer

Elsevier Information Systems GmbH
Franklinstr. 61-63
60486 Frankfurt am Main
Germany
Phone: +49 69 5050 4242

Copyright Holder:
Elsevier Properties SA
Espace de l'Europe 3
CH-2000, Neuchâtel
Switzerland

Sources

- More than 16,000 chemistry-related periodicals
- Conference abstracts
- Patent information from all major authorities

User Aids

- Online Helps (HELP DIRECTORY lists all help messages available)
- STNGUIDE

Clusters

- CASRNS
- STRUCTURE

STN Database Cluster information

Related Databases

REAXYSFILEBIB

Search and Display Field Codes

Fields that allow left truncation are indicated by an asterisk (*).

Search Field Name	Search Code	Search Examples	Display Codes
Basic Index* (contains single terms from Chemical Name (CN) and Chemical Name Segment (CNS))	/BI	S CINNAMON? AND ACID S URIDIN? AND HYDROXY?/BI S URIDINE/BI	CN, CNS
Accession Number	/AN	S 1915876/AN	AN
All Accession Numbers	/ALLAN	S 1915876/ALLAN	AN, CMAN, COMPAN
CAS Registry Number	/RN	S 100-03-8/RN	RN
Chemical Name	/CN	S CHOLESTEROL/CN	CN
Chemical Name Segment*	/CNS	S ?CHOLESTERYL/CNS	CN
Component Molecular Accession Number	/CMAN	S 5811/CMAN	CMAN
Component Molecular Formula	/CMF	S C6 H13 N/CMF	CMF
Composition Accession Number	/COMPAN	S 8181997/COMPAN	COMPAN
Composition Concentration	/COMPC	S B WEIGHT PERCENT/COMPC	COMPC
Composition Name	/COMPN	S CHROMIUM/COMPN	COMPN
Count of Referenced Markush Structures **(1)**	/MARKREF.CNT	S 10/MARKREF.CNT	MARKREF.CNT
Element Count, Substance **(1)**	/ELC.SUB	S AU/ELS AND 5/ELC.SUB	MF
Element Symbol **(2)**	/ELS	S CL/ELS	MF
Element Symbol, Count **(1)**	/ELS.CNT	S 5/ELS.CNT	MF
Entry Date **(1)**	/ED	S L1 AND ED=JUL 2020	ED
Field Availability **(3)**	/FA	S SD/FA	Not displayed
Field Availability, Properties **(4)**	/FA.P	S BP/FA.P S BOILING POINT/FA.P	FA.P
Field Availability, Reactions	/FA.RX	S RX.PAN/FA.RX	FA.RX
Molecular Weight **(1)**	/MW (or /FW)	S 3000<FW S 100-200/MW	MW
InChi Key	/INCHI (or /INKY)	S KWEZFXJCZZEGTG-JGRHXJNXSA-N/INCHI	INCHI
Linearized Structure Formula	/LSF	S "CH2O(1+)"/LSF	LSF
Molecular Formula	/MF	S C4H9N5/MF	MF
Number of Components **(1)**	/NC	S 9/NC	NC
Periodic Group	/PG	S (A3 AND A6)/PG	MF
Reference Count **(1)**	/REC	S REC>=15	REC
Reaction ALL Accession Numbers **(5)**	/RX.AAN	S 11993319/RX.AAN	RX
Reaction Catalyst Accession Number **(5)**	/RX.CAAN	S 13182466/RX.CAAN	RX
Reaction Classification **(5)**	/RX.CL	S PREPARATION/RX.CL	RX
Reaction Product Accession Number **(5)**	/RX.PAN	S 11993319/RX.PAN	RX
Reaction Product Accession Number (Details) **(5)**	/RX.PRAN	S 21007747/RX.PRAN	RX
Reaction Product **(5)**	/RX.PRO	S FORMALDEHYDE/RX.PRO	RX
Reaction Reactant Accession Number **(5)**	/RX.RAN	S 5678943/RX.RAN S 1000/RX.PAN (P) 6831972/RX.RAN S 1000/RX.RAN (P) REPARATION/RX.CL	RX RX
Reaction Reagent Accession Number (Details) **(5)**	/RX.RGAN (or /RX RCAN)	S 105690/RX.RGAN	RX
Reaction Reactant **(5)**	/RX.RCT	S SULFURIC ACID/RX.RCT	RX
Reaction Solvent Accession Number **(5)**	/RX.SOLAN	S 1696894/RX.SOLAN	RX

Search and Display Field Codes (cont'd)

Search Field Name	Search Code	Search Examples	Display Codes
Substance Descriptor Update Date **(1)**	/SD /UP	S ISOCYCLIC/SD S L1 AND UP>= JAN 2024	SD UP

(1) Numeric search field that may be searched using numeric operators or ranges.
(2) Search with implied(S) proximity is available in this field.
(3) Field AINCHI no more available as of February 2026.
(4) For details on Searching Properties, see Table “Searching Properties” on page 3.
(5) P-proximity is used to retrieve, e.g., reactant and product, from the same reaction.

Searching Properties

Properties may be searched in Field Availability, Properties (/FA.P) by using name or code – see table below.

Property Type	Name	Code	Search Examples	Display Code
Physical Property	Boiling Point	BP	S BP/FA.p	BP
	Bulk Viscosity	BV	S BV/FA.P	BV
	Critical Micelle Concentration	CMC	S CMC/FA.P	CMC
	Density of the Liquid	DEN	S DEN/FA.P	DEN
	Dielectric Constant	DIC	S DIC/FA.P	DIC
	Dissociation Energy	EDIS	S EDIS/FA.P	EDIS
	Dissociation Exponent	DE	S DE/FA.P	DE
	Dynamic Viscosity	DV	S DV/FA.P	DV
	Electrical Data	ELE	S ELE/FA.P	ELE
	Electrical Moment	EM	S EM/FA.P	EM
	Electrolytic Conductivity	ELYC	S ELYC/FA.P	ELYC
	Energy Barriers	EBC	S EBC/FA.P	EBC
	Enthalpies of Other Phase Transitions	HPT	S HPT/FA.P	HPT
	Enthalpy of Combustion	HCOM	S HCOM/FA.P	HCOM
	Enthalpy of Formation	HFOR	S HFOR/FA.P	HFOR
	Enthalpy of Fusion	HFUS	S HFUS/FA.P	HFUS
	Enthalpy of Hydrogenation	HHDG	S HHDG/FA.P	HHDG
	Enthalpy of Sublimation	HSB	S HSB/FA.P	HSB
	Enthalpy of Vaporization	HVAP	S HVAP/FA.P	HVAP
	Flash Point	FP	S FP/FA.P	FP
	Heat Capacity Cp	CP	S CP/FA.P	CP
	Heat Capacity Cp0	CP0	S CP0/FA.P	CP0
	Heat Capacity Cv	CV	S CV/FA.P	CV
	Henry Constant	HNC	S HNC/FA.P	HNC
	Ionization Potential	IP	S IP/FA.P	IP
	Isoelectric Point	IEP	S IEP/FA.P	IEP
	Kinematic Viscosity	KV	S KV/FA.P	KV
	Liquid/Vapor Systems	LVSM	S LVSM/FA.P	LVSM
	Magnetic Susceptibility	MSUS	S MSUS/FA.P	MSUS
	Melting Point	MP	S MP/FA.P	MP
	Mutarotation	MUT	S MUT/FA.P	MUT
	Optical Rotatory Power	ORP	S ORP/FA.P	ORP
	Partition Octan-1-Ol/Water	POW	S POW/FA.P	POW
	Refractive Index	RI	S RI/FA.P	RI
	Self-Diffusion Coefficient	SDIF	S SDIF/FA.P	SDIF
	Solubility	SLB	S SLB/FA.P	SLB
	Solubility Product	SLBP	S SLBP/FA.P	SLBP
	Static Dielectric Constant	SDIC	S SDIC/FA.P	SDIC
	Sublimation	SP	S SP/FA.P	SP
	Surface Tension	ST	S ST/FA.P	ST
	Thermal Expansion	TEC	S TEC/FA.P	TEC
	Vapor Pressure	VP	S VP//FA.P	VP

Searching Properties (cont'd)

Property Type	Name	Code	Search Examples	Display Code
Aggregation State	Critical Density	CRD	S CRD/FA.P	CRD
	Critical Pressure	CRP	S CRP/FA.P	CRP
	Critical Temperature	CRT	S CRT/FA.P	CRT
	Critical Volume	CRV	S CRV/FA.P	CRV
	Crystal Phase	CRYPH	S CRYPH/FA.P	CRYPH
	Crystal Phase Transition Point	CPTP	S CPTP/FA.P	CPTP
	Crystal Property Description	CPD	S CPD/FA.P	CPD
	Crystal Space Group	CSG	S CSG/FA.P	CSG
	Crystal System	CSYS	S CSYS/FA.P	CSYS
	Decomposition Point	DP	S DP/FA.P	DP
	Gas Phase	GP	S GP/FA.P	GP
	Liquid Phase	LQPH	S LQPH/FA.P	LQPH
	Transition Point(s) of Liquid Modification	LPTP	S LPTP/FA.P	LPTP
	Triple Point	TP	S TP/FA.P	TP
Spectroscopy	ESR Spectroscopy	ESR	S ESR/FA.P	ESR
	Fluorescence Spectroscopy	FLUS	S FLUS/FA.P	FLUS
	IR Spectroscopy	IR	S IR/FA.P	IR
	Luminescence Spectroscopy	LUM	S LUM/FA.P	LUM
	Mass Spectrometry	MS	S MS/FA.P	MS
	NMR Spectroscopy	NMR	S NMR/FA.P	NMR
	NQR Spectroscopy	NQR	S NQR/FA.P	NQR
	Other Spectroscopic Methods	OSM	S OSM/FA.P	OSM
	Phosphorescence Spectroscopy	PHOS	S PHOS/FA.P	PHOS
	Raman Spectroscopy	RAS	S RAS/FA.P	RAS
	Rotational Spectroscopy	ROT	S ROT/FA.P	ROT
	UV/VIS Spectroscopy	UVS	S UVS/FA.P	UVS
Multi-Component System	Adsorption	DSM	S ADSM/FA.P	DSM
	Associations	ASSM	S ASSM/FA.P	ASSM
	Azeotropes	AZE	S AZE/FA.P	AZE
	Boundary Surface Phenomena	BSPM	S BSPM/FA.P	BSPM
	Complex Phase Equilibria	CPEM	S CPEM/FA.P	CPEM
	Electrical Data	EDM	S EDM/FA.P	EDM
	Energy Data	ENEM	S ENEM/FA.P	ENEM
	Liquid/Liquid Systems	LLSM	S LLSM/FA.P	LLSM
	Liquid/Solid Systems	LSSM	S LSSM/FA.P	LSSM
	Liquid/Vapor Systems	LVSM	S LVSM/FA.P	LVSM
	Mechanical and Physical Properties	MECM	S MECM/FA.P	MECM
	Optical Data	ODM	S ODM/FA.P	ODM
	Partition octan-1-ol/water	POW	S POW/FA.P	POW
	Solution Behavior	SOLM	S SOLM/FA.P	SOLM
	Transport Phenomena	TRAM	S TRAM/FA.P	TRAM
Further Properties	Acoustic Properties	SOUND	S SOUND/FA.P	SOUND
	Autoignition	AIT	S AIT/FA.P	AIT
	Chemical Derivative	CDER	S CDER/FA.P	CDER
	Circular Dichroism	CDIC	S CDIC/FA.P	CDIC
	Compressibility	CMP	S CMP/FA.P	CMP
	Conformation	CNF	S CNF/FA.P	CNF
	Cross-Sections	XS	S XS/FA.P	XS
	Electrical Polarizability	ELP	S ELP/FA.P	ELP
	Electrochemical Behavior	ELCB	S ELCB/FA.P	ELCB
	Electrochemical Characteristics	POT	S POT/FA.P	POT
	Electrochemical Data	ELCH	S ELCH/FA.P	ELCH
	Electron Binding	CIP	S CIP/FA.P	CIP
	Explosion Limits	EL	S EL/FA.P	EL
	Further Information	FINFO	S FINFO/FA.P	FINFO
	Further Information	FINFO1	S FINFO1/FA.P	FINFO1
	Further Information	FINFO2	S FINFO2/FA.P	FINFO2
	Further Information	FINFO3	S FINFO3/FA.P	FINFO3
	Interatomic Distances and Angles	IDA	S IDA/FA.P	IDA
	Isolation from Natural Product	INP	S INP/FA.P	INP

Searching Properties (cont'd)

Property Type	Name	Code	Search Examples	Display Code
	Magnetic Data	MAG	S MAG/FA.P	MAG
	Mechanical Properties	MEC	S MEC/FA.P	MEC
	Molecular Deformation	DFM	S DFM/FA.P	DFM
	Optical Rotatory Dispersion	ORD	S ORD/FA.P	ORD
	Optics	OPT	S OPT/FA.P	OPT
	Other Thermochemical Data	OTHE	S OTHE/FA.P	OTHE
	Patent Specific Data	PSD	S PSD/FA.P	PSD
	Purification	PUR	S PUR/FA.P	PUR
	Quantum Chemical Calculations	QCC	S QCC/FA.P	QCC
	Related Structure	RSTR	S RSTR/FA.P	RSTR
	Substance Label	LB	S LB/FA.P	LB
	Transport Data	TRAN	S TRAN/FA.P	TRAN

Structure Searching - Structure Search Terms

Terms	Search Examples
L-numbers of structures uploaded from the STNext structure editor (Boolean logic allowed between the L-numbers)	SEARCH L1 FAM SAM SEA L1 AND L2 SSS FUL

Types of Structure Searching

Type	Definition	Search Code	Search Examples
Substructure (default)	Search for substances which match the query. Substitution is allowed at all open positions. Additional components may be retrieved	SSS	SEARCH L1 SSS FUL S L2 OR L3 SSS SAM S L7 SSS RAN
Closed Substructure	Search for substances which match the query exactly. Substitution is allowed at positions by assigning non-hydrogen attachments. Right click on a node or group of nodes and use the Non-Hydrogen Count tab in the STNext structure drawing tool. Additional components may be retrieved.	CSS	SEARCH L1 CSS FUL S L2 OR L3 CSS S L4 NOT L5 CSS RAN
Family	Search for substances which match the query exactly. Additional components may be retrieved.	FAM	S L6 FAM SAM
Exact	Search for substances which match the query exactly.	EXA	SEA L5 EXA FUL

Scopes of Structure Searches

Type	Definition	Search Code	Search Examples
Sample (default)	Search a fixed 5% of the file	SAM	SEARCH L3 EXA SAM S L6 NOT L7 SSS SAM
Full	Search 100% of the file.	FUL	S L5 OR L8 SSS FUL

DISPLAY and PRINT Formats

Any combination of formats may be used to display or print answers. Multiple codes must be separated by spaces or commas, e.g., D L1 1-5 TI AU. The fields are displayed or printed in the order requested. Hit term highlighting is available for all fields. Highlighting must be ON during SEARCH to use the HIT, KWIC, and OCC formats.

SET LINE 150 is recommended for display of property tables.

Format	Content	Examples
AN	Accession Number	D AN
CMAN	Component Molecular Accession Number	D CMAN
CMF	Component Molecular Formula	D CMF
CN	Chemical Name	D CN
COMPAN	Composition Accession Number	D COMPAN
COMPN	Composition Concentration	D COMPN
ED	Entry Date	D ED
FA.P	Field Availability, Properties	D FA.P
FA.RX	Field Availability, Reactions	D FA.RX
INCHI (INKY)	InChi Key	D INCHI
LSF	Linearized Structure Formula	D LSF
MARKREF.CNT	Count of Referenced Markush Structures	D MARKREF.CNT
MF	Molecular Formula	D MF
MW	Molecular Weight	D MW
PG	Periodic Group	D PG
REC (RE.CNT)	Reference Count	D REC
RN	CAS Registry Number	D RN
SD	Substance Descriptor	D SD
STR	Structure	D STR
UP	Update Date	D UP
PHYS **(3)**	All Physical Properties	D PHYS
STATE **(3)**	All Aggregation State Properties	D STATE
FURTHER **(3)**	All Further Properties	D FURTHER
MULTI **(3)**	All Multicomponent Properties	D MULTI
SPEC **(3)**	All Spectroscopy Properties	D SPEC
ALL	AN, CN, SD, COMPAN, COMPN, COMPC, MF, CMF, LSF, INCHI, MW, MARKREF.CNT, REC, ED, UP, STR, PROPERTIES, FA.P, FA.RX, RX.ID, RX.PAN, RX.RAN	D ALL
IALL	ALL, indented with text labels	D IALL
IDE	AN, CN, SD, COMPAN, COMPN, COMPC, MF, CMF, LSF, INCHI, MW, MARKREF.CNT, REC, ED, UP, STR	D IDE
QRD **(1)**	Query Related Data (default)	D QRD
SCAN **(2)**	CN, MF, SD, STR (random display, no answer number)	D SCAN
SAM, SAMPLE	AN, CN, MF, SD, STR	D SAMPLE
HIT	All fields containing hit terms	D HIT
HIT IDE	Complete IDE with HIT	D HIT IDE
PROP	All Properties	D PROP
RX	All Reactions Data	D RX

(1) Default: Dynamic display format QRD (Query Related Data) providing information on Identification of Substance (IDE) plus those display fields in which your search terms appear (HIT).
(2) SCAN must be specified on the command line, i.e., D SCAN or DISPLAY SCAN.
(3) Displays all individual properties available within this group. For streamlined data content and more predictable pricing, consider DISPLAY QRD.

SELECT, ANALYZE, and SORT Fields

The SELECT command is used to create E-numbers containing terms taken from the specified field in an answer set.

The ANALYZE command is used to create an L-number containing terms taken from the specified field in an answer set.

The SORT command is used to rearrange the search results in either alphabetic or numeric order of the specified field(s).

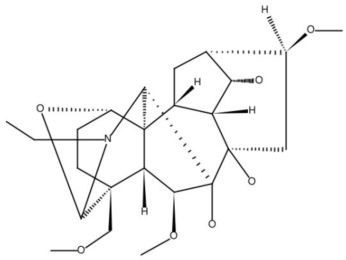
Field Name	Field Code	ANALYZE/ SELECT (1)	SORT
Accession Number	AN	Y	Y
Chemical Name	CN	Y	N
InCHi Key	INCHI (INKY)	Y	Y
Molecular Weight	MW	N	Y
Number of Components	NC	N	Y
Reference Count	RE (RE.CNT)	N	Y
CAS Registry Number	RN	Y	N
All Accession Numbers from reaction document	RX.AAN	Y	N
Reaction Catalyst Accession Number	RX.CAAN	Y	N
Reaction Product Accession Number	RX.PAN	Y	N
Reaction Product Accession Number (Details)	RX.PRAN	Y	N
Reaction Reactant Accession Number	RX.RAN	Y	N
Reaction Reagent Accession Number (Details)	RX.RGAN (RX.RCAN)	Y	N
Reaction Solvent Accession Number	RX.SOLAN	Y	N
Substance Descriptor	SD	Y	N

(1) HIT may be used to restrict terms extracted to terms that match the search expression used to create the answer set, e.g., SEL HIT RN.

SAMPLE Records

Display ALL

```
AN      54944   REAXYSFILESU
RN      85649-35-0
CN      (16(i)S)-20-ethyl-13B1; ,19-epoxy-63B2;
        ,16-dimethoxy-4-methoxymethyl-aconitane-7,8,143B1; -triol;
        (16(i)S)-20-Aethyl-13B1; ,19-epoxy-63B2;
        ,16-dimethoxy-4-methoxymethyl-aconitan-7,8,143B1; -triol
SD      heterocyclic
MF      C24 H37 N O7
CMF     C24 H37 N O7
LSF     C24H37NO7
INCHI   NUULWSXOCUBEST-ZLLQYLGQSA-N
MW      451.56
MARKREF.CNT 0
REC     2
ED      Entered STN: 14 Jul 2020
        Last updated on STN: 19 Jan 2024
```



```
PROPERTIES
        DE Dissociation Exponent  (1) (PHYS)
        MP Melting Point (1) (PHYS)
        ORP Optical Rotatory Power (1) (PHYS)
FA.RX   RX.ID; RX.PAN; RX.RAN   (6)
```

Display RX PROP

L4 ANSWER 1 OF 1 REAXYSFILESU COPYRIGHT 2025 ELSEVIER INC. on STN.

Reaction:

Reaction ID:	22271502
Reactant AN (.RAN):	54944
Reactant (.RCT):	(16<i>S)-20-ethyl-13B1;,19-epoxy-63B2;,16-dimethoxy-4-methoxymethyl-aconitane-7,8,143B1;-triol
Product AN (.PAN):	68455
Product (.PRO):	(8<i>S)-143B1;-acetoxy-20-ethyl-13B1;,8-epoxy-8-hydroxy-63B2;-methoxy-4-methoxymethyl-7,8-seco-aconitane-7,19-dione
Reference Count:	1

Reaction Details:

Reaction RID:	22271502.1
Reaction Classification (.CL):	Multi-step reaction
Reagent AN (.RGAN):	11343348; 11378922; 2037554; 3587155; 506007; 5327449; 635680
Reagent:	potassium permanganate; palladium on activated charcoal; sulfuric acid; water; acetic acid; periodic acid; acetone
Reference(s):	761525: Journal: Anet et al., Can. J. Chem. (1958) Vol. 36, 766,769p.

Reaction:

Reaction ID:	22271501
Reactant AN (.RAN):	54944
Reactant (.RCT):	(16<i>S)-20-ethyl-13B1;,19-epoxy-63B2;,16-dimethoxy-4-methoxymethyl-aconitane-7,8,143B1;-triol
Product AN (.PAN):	66524
Product (.PRO):	143B1;-acetoxy-20-ethyl-13B1;,19-epoxy-63B2;-methoxy-4-methoxymethyl-7,8-seco-aconit-15-ene-7,8-dione
Reference Count:	1

Reaction Details:

Reaction RID:	22271501.1
Reaction Classification (.CL):	Multi-step reaction
Reagent AN (.RGAN):	2037554; 506007; 5327449
Reagent:	sulfuric acid; acetic acid; periodic acid
Reference(s):	761525: Journal: Anet et al., Can. J. Chem. (1958) Vol. 36, 766,769p.

Reaction:

Reaction ID:	22271500
Reactant AN (.RAN):	54944
Reactant (.RCT):	(16<i>S)-20-ethyl-13B1;,19-epoxy-63B2;,16-dimethoxy-4-methoxymethyl-aconitane-7,8,143B1;-triol
Product AN (.PAN):	64526
Product (.PRO):	(8<i>S)-143B1;-acetoxy-20-ethyl-13B1;,8-epoxy-8-hydroxy-63B2;-methoxy-4-methoxymethyl-7,8-seco-aconitan-7-one
Reference Count:	1

Reaction Details:

Reaction RID:	22271500.1
Reaction Classification (.CL):	Multi-step reaction
Reagent AN (.RGAN):	11378922; 2037554; 3587155; 506007; 5327449

```
       Reagent:                        palladium on activated charcoal; sulfuric
                                       acid; water; acetic acid; periodic acid
       Reference(s):                   761525: Journal: Anet et al., Can. J.
                                       Chem. (1958) Vol. 36, 766,769p.

Reaction:
       Reaction ID:                    5739558
       Reactant AN (.RAN):             52318
       Reactant (.RCT):                delcosine
       Product AN (.PAN):              54944
       Product (.PRO):                 (16<i>S)-20-ethyl-13B1;,19-epoxy-63B2;,16-
                                       dimethoxy-4-methoxymethyl-aconitane-7,8,1
                                       43B1;-triol; <i>N-deethyl-delcosine
       Reference Count:                1


Reaction Details:
       Reaction RID:                   5739558.1
       Reaction Classification (.CL): Preparation
       Reagent AN (.RGAN):             113916; 635680
       Reagent:                        N-Bromosuccinimide; acetone
       Reference(s):                   1034996: Journal: Ant al. et al., Can. J.
                                       Chem. (1957) Vol. 35, 397,402p.

Reaction:
       Reaction ID:                    675288
       Reactant AN (.RAN):             52318
       Reactant (.RCT):                delcosine
       Product AN (.PAN):              54944
       Product (.PRO):                 (16<i>S)-20-ethyl-13B1;,19-epoxy-63B2;,16-
                                       dimethoxy-4-methoxymethyl-aconitane-7,8,1
                                       43B1;-triol
       Reference Count:                1


Reaction Details:
       Reaction RID:                   675288.1
       Reaction Classification (.CL): Preparation
       Reagent AN (.RGAN):             3595636; 506007
       Reagent:                        silver(I) acetate; acetic acid
       Reference(s):                   1034996: Journal: Ant al. et al., Can. J.
                                       Chem. (1957) Vol. 35, 397,402p.

Reaction:
       Reaction ID:                    677086
       Reactant AN (.RAN):             54944
       Reactant (.RCT):                (16<i>S)-20-ethyl-13B1;,19-epoxy-63B2;,16-
                                       dimethoxy-4-methoxymethyl-aconitane-7,8,1
                                       43B1;-triol
       Product AN (.PAN):              69896
       Product (.PRO):                 (16<i>S)-143B1;-acetoxy-20-ethyl-13B1;,19-
                                       epoxy-63B2;,16-dimethoxy-4-methoxymethyl-
                                       7,8-seco-aconitane-7,8-dione
       Reference Count:                1


Reaction Details:
       Reaction RID:                   677086.1
       Reaction Classification (.CL): Preparation
       Reagent AN (.RGAN):             5327449
       Reagent:                        periodic acid
       Reference(s):                   761525: Journal: Anet et al., Can. J.
                                       Chem. (1958) Vol. 36, 766,769p.
AN     54944   REAXYSFILESU

Dissociation Exponent  (1)
 Value      | Method         | Solvent     | Type       | Ref(s)
```

(DE) (--)	(.MET)	(.SOL)	(.TYP)	(REF)
4.2	potentiometric	aq. ethanol	a/apparent	1

1. AN 1034996: Journal: Ant al. et al., Can. J. Chem. (1957) Vol. 35, 397,402p.

Melting Point (1)

Value (MP) (Cel)	Solvent (.SOL)	Ref(s) (REF)
188 - 189	acetone; petroleum ether	1

1. AN 1034996: Journal: Ant al. et al., Can. J. Chem. (1957) Vol. 35, 397,402p.

Optical Rotatory Power (1)

Part 1 of 2 | Value (ORP) (deg)	Concentr. (.C)	Solvent (.SOL)	Temp. (.T) (Cel)	Type (.TYP)
1 | 74.6	c=1.4	CHCl3	22	[alpha]

Optical Rotatory Power (1)

Part 2 of 2 | Wavelength (.W) (nm)	Ref(s) (REF)
1 | 589	1

1. AN 1034996: Journal: Ant al. et al., Can. J. Chem. (1957) Vol. 35, 397,402p.

In North America

CAS Customer Center:
P.O. Box 3012
Columbus, Ohio 43210-0012
U.S.A.

Phone: 800-753-4227 (North America)
614-447-3731 (worldwide)
E-mail: help@cas.org
Internet: www.cas.org

In Europe

CAS Customer Center EMEA
represented by
FIZ Karlsruhe - Leibniz-Institute for Information Infrastructure
Hermann-von-Helmholtz-Platz 1
76344 Eggenstein-Leopoldshafen
Germany

Phone: +49-721-9588 3155
E-mail: EMEAhelp@cas.org
Internet: www.fiz-karlsruhe.de

In Japan

JAICI
(Japan Association for International Chemical Information)
Nakai Building
6-25-4 Honkomagome, Bunkyo-ku
Tokyo 113-0021
Japan

Phone: +81-3-5978-3601 (Technical Service)
+81-3-5978-3621 (Customer Service)
E-mail: support@jaici.or.jp (Technical Service)
customer@jaici.or.jp (Customer Service)
Internet: www.jaici.or.jp